

Experimental Mathematics and the Normality of Pi

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Computers in Mathematics



Although the computer's origin was in the field of pure mathematics (Turing, Von Neumann, others), computer technology has heretofore played a relatively minor role in mathematical research.

A sea change is now underway:

- Powerful, broad-spectrum mathematical computing software, especially Mathematica and Maple.
- High-precision computation facilities.
- Useful Internet-based facilities, particularly for sequence and constant recognition.
- Advanced visualization tools.
- A new generation of mathematicians, raised in the computer age, eagerly using these new tools.

Experimental Mathematics



The computer has in turn changed the very nature of mathematical experience, suggesting for the first time that mathematics, like physics, may yet become an empirical discipline, a place where things are discovered because they are seen.

David Berlinski, 1997

If mathematics describes an objective world just like physics, there is no reason why inductive methods should not be applied in mathematics just the same as in physics.

Kurt Godel, 1951

The Computer-Experimental Methodology in Mathematics



- Gaining insight and intuition.
- Discovering new patterns and relationships.
- Using graphical displays to suggest underlying mathematical principles.
- Testing and especially falsifying conjectures.
- Exploring a possible result to see if it is worth formal proof.
- Suggesting approaches for formal proof.
- Replacing lengthy hand derivations with computerbased derivations.
- Confirming analytically derived results.

Experimental Math in Action



In 1988, Joseph Roy North observed that Gregory's series,

$$\pi = 4(1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \frac{1}{9} - \frac{1}{11} + \cdots)$$

when truncated to 5,000,000 terms, gives a value that differs strangely from the true value of π :

Sloane's Encyclopedia of Integer Sequences, available at http://www.research.att.com/~njas/sequences recognizes these integers as Euler numbers E_n. The above phenomenon is an artifact of the fact that 5,000,000 is one-half of a large power of ten.

The PSLQ Integer Relation Algorithm



Let (x_n) be a vector of real numbers. An integer relation algorithm finds integers (a_n) such that

$$a_1x_1 + a_2x_2 + \dots + a_nx_n = 0$$

- At the present time, the PSLQ algorithm of Helaman Ferguson is the best algorithm for integer relation detection.
- PSLQ was named one of ten "algorithms of the century" by Computing in Science and Engineering.
- High precision arithmetic software is required:
 At least d § n digits, where d is the size (in digits) of the largest of the integers a_k.

Ferguson's "Eight-Fold Way" Sculpture





LBNL's Arbitrary Precision Computation (ARPREC) Package



- Low-level routines written in C++.
- C++ and F-90 translation modules permit use with existing programs with only minor code changes.
- Double-double (32 digits), quad-double, (64 digits) and arbitrary precision (>64 digits) available.
- Special routines for extra-high precision (>1000 dig).
- Includes common math functions: sqrt, cos, exp, etc.
- PSLQ, root finding, numerical integration.

Authors: Brandon Thompson (Stanford), Sherry Li (LBNL), Yozo Hida (UCB) and DHB.

Available at: http://www.expmath.info

The Experimental Mathematician's Toolkit



- An interactive tool for high-precision experimental math calculations, based on ARPREC.
- Features include:
 - General arithmetic expressions.
 - Number theory functions: binomial, factorial, etc.
 - Transcendental functions: sqrt, cos, exp, arctan, erf, etc.
 - PSLQ.
 - Polynomial root finding.
 - Definite integrals (ie, numerical quadrature).
 - Summations (infinite series).
- Soon to be made available as a web-based tool.

Available at: http://www.expmath.info

Identifying Algebraic Numbers Using PSLQ



Problem: Is a given real number α algebraic of degree n or less? I.e., is α the root of an algebraic equation with integer coefficients of degree n or less?

Solution: Compute the set of numbers

$$(1, \alpha, \alpha^2, \alpha^3, \cdots, \alpha^n)$$

to high precision, and then apply PSLQ.

Example (using Mathematician's Toolkit):

$$0 = 1 - 3860t^4 - 666t^8 - 20t^{12} + t^{16}$$

Bifurcation Points in Chaos Theory



 $B_3 = 3.54409035955...$ is third bifurcation point of the logistic iteration of chaos theory:

$$x_{n+1} = rx_n(1-x_n)$$

i.e., B₃ is the smallest r such that the iteration exhibits 8-way periodicity instead of 4-way periodicity.

PSLQ can determine that B₃ satisfies

$$0 = 4913 + 2108t^{2} - 604t^{3} - 977t^{4} + 8t^{5} + 44t^{6} + 392t^{7}$$
$$-193t^{8} - 40t^{9} + 48t^{10} - 12t^{11} + t^{12}$$

Recently B₄ was identified as the root of a 256-degree polynomial (a much more challenging computation).

These results have subsequently been proven formally.

Fascination With Pi



Newton (1670):

"I am ashamed to tell you to how many figures I carried these computations, having no other business at the time."



 In his book "Contact," the lead scientist (played by Jodie Foster in the movie) looked for patterns in the digits of pi.





Carl E. Sagan

Fax from "The Simpsons" Show







Banned by 20th **Century Fox**

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PHONE (310) 203-3959

A frofessor at UCLA told me that you might be able to give me the you might be able to give me the answer to: What is the 40,000 the digit of fi?

We would like to use the answer?

In our show. Can you help?

Peter Borwein's Observation



In 1996, Peter Borwein of SFU in Canada observed that the following well-known formula for log_e 2

$$\log 2 = \sum_{n=1}^{\infty} \frac{1}{n2^n} = 0.69314718055994530942...$$

leads to a simple scheme for computing binary digits at an arbitrary starting position (here {} denotes fractional part):

$$\left\{2^{d} \log 2\right\} = \left\{\sum_{n=1}^{d} \frac{2^{d-n}}{n}\right\} + \sum_{n=d+1}^{\infty} \frac{2^{d-n}}{n} \\
= \left\{\sum_{n=1}^{d} \frac{2^{d-n} \bmod n}{n}\right\} + \sum_{n=d+1}^{\infty} \frac{2^{d-n}}{n}$$

Fast Exponentiation



The exponentiation (2^{d-n} mod n) in this formula can be evaluated very rapidly by means of the binary algorithm for exponentiation, performed modulo n:

Example:

$$3^{17} = (((3^2)^2)^2)^2 \times 3 = 129140163$$

In a similar way, we can evaluate:

```
3^{17} \mod 10 = ((((3^2 \mod 10)^2 \mod 10)^2 \mod 10)^2 \mod 10) \times 3 \mod 10
3^2 \mod 10 = 9
```

 $9^2 \mod 10 = 1$

 $1^2 \mod 10 = 1$

 $1^2 \mod 10 = 1$

 $1 \times 3 = 3$ Thus $3^{17} \mod 10 = 3$.

Note: we never have to deal with integers larger than 81.

Is There an Arbitrary Digit Calculation Formula for Pi?



The same trick can be used for any mathematical constant given by a formula of the form

$$\alpha = \sum_{n=1}^{\infty} \frac{p(n)}{q(n)2^n}$$

where p and q are polynomials with integer coefficients, deg p < q, and q has no zeroes at positive integers. Any linear sum of such constants also has this property.

Is there a formula of this type for π ? Until recently, none was known in mathematical literature.

The BBP Formula for Pi



In 1996, a PSLQ program discovered this formula for pi:

$$\pi = \sum_{k=0}^{\infty} \frac{1}{16^k} \left(\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6} \right)$$

Indeed, this formula permits one to directly calculate binary or hexadecimal (base-16) digits of π beginning at an arbitrary starting position n, without needing to calculate any of the first n-1 digits.

So simple! Why wasn't it found hundreds of years ago? Answer: Maybe it had to await the computer age – until recently no one would have thought to seek such a formula.

Proof of the BBP Formula



$$\int_0^{1/\sqrt{2}} \frac{x^{j-1} dx}{1 - x^8} = \int_0^{1/\sqrt{2}} \sum_{k=0}^{\infty} x^{8k+j-1} dx = \frac{1}{2^{j/2}} \sum_{k=0}^{\infty} \frac{1}{16^k (8k+j)}$$

Thus

$$\sum_{k=0}^{\infty} \frac{1}{16^k} \left(\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6} \right)$$

$$= \int_0^{1/\sqrt{2}} \frac{(4\sqrt{2} - 8x^3 - 4\sqrt{2}x^4 - 8x^5) dx}{1 - x^8}$$

$$= \int_0^1 \frac{16(4 - 2y^3 - y^4 - y^5) dy}{16 - y^8}$$

$$= \int_0^1 \frac{16(y - 1) dy}{(y^2 - 2)(y^2 - 2y + 2)}$$

$$= \int_0^1 \frac{4y dy}{y^2 - 2} - \int_0^1 \frac{(4y - 8) dy}{y^2 - 2y + 2}$$

$$= \pi$$

Algorithm for Computing Hex Digits of Pi Starting After d Digits



Let S_1 be the first of the four sums in the formula for π . Then the hex expansion of S_1 beginning after position d is:

$$\begin{cases}
16^{d}S_{1}\} = \left\{ \sum_{k=0}^{\infty} \frac{16^{d-k}}{8k+1} \right\} = \left\{ \sum_{k=0}^{d} \frac{16^{d-k}}{8k+1} \right\} + \sum_{k=d+1}^{\infty} \frac{16^{d-k}}{8k+1} \\
= \left\{ \sum_{k=0}^{n} \frac{16^{n-k} \mod 8k+1}{8k+1} \right\} + \sum_{k=n+1}^{\infty} \frac{16^{n-k}}{8k+1}
\end{cases}$$

The numerator of the first summation can be evaluated very rapidly using the binary algorithm for exponentiation, performed mod 8k+1. Only a few terms of the second sum need to be calculated, since it converges rapidly. Repeat for S_1 , S_2 , S_3 , S_4 and combine according to the BBP formula. The final fraction, expressed in hexadecimal format, is the desired string.

The entire algorithm may be performed with ordinary 64-bit or 128-bit floating-point arithmetic.

Calculations Using the BBP Algorithm



Position	Hex Digits of Pi	Starting at Position
	9	9

10⁶ 26C65E52CB4593

10⁷ 17AF5863EFED8D

10⁸ ECB840E21926EC

10⁹ 85895585A0428B

10¹⁰ 921C73C6838FB2

10¹¹ 9C381872D27596

1.25 x 10¹² 07E45733CC790B **[1]**

2.5 x 10¹⁴ E6216B069CB6C1 [2]

- [1] Babrice Bellard, France, 1999
- [2] Colin Percival, Canada, 2000

Some Other New Math Identities



$$\pi\sqrt{3} = \frac{9}{32} \sum_{k=0}^{\infty} \frac{1}{64^k} \left(\frac{16}{6k+1} - \frac{8}{6k+2} - \frac{2}{6k+4} - \frac{1}{6k+5} \right)$$

$$\pi^2 = \frac{1}{8} \sum_{k=0}^{\infty} \frac{1}{64^k} \left(\frac{144}{(6k+1)^2} - \frac{216}{(6k+2)^2} - \frac{72}{(6k+3)^2} - \frac{54}{(6k+4)^2} + \frac{9}{(6k+5)^2} \right)$$

$$\pi^2 = \frac{2}{27} \sum_{k=0}^{\infty} \frac{1}{729^k} \left(\frac{243}{(12k+1)^2} - \frac{405}{(12k+2)^2} - \frac{81}{(12k+4)^2} - \frac{27}{(12k+5)^2} \right)$$

$$-\frac{72}{(12k+6)^2} - \frac{9}{(12k+7)^2} - \frac{9}{(12k+8)^2} - \frac{5}{(12k+10)^2} + \frac{1}{(12k+11)^2} \right)$$

$$6\sqrt{3} \arctan\left(\frac{\sqrt{3}}{7}\right) = \sum_{k=0}^{\infty} \frac{1}{27^k} \left(\frac{3}{3k+1} + \frac{1}{3k+2}\right)$$

$$\frac{25}{2} \log\left(\frac{781}{256} \left(\frac{57 - 5\sqrt{5}}{57 + 5\sqrt{5}}\right)^{\sqrt{5}}\right) = \sum_{k=0}^{\infty} \frac{1}{55^k} \left(\frac{5}{5k+2} + \frac{1}{5k+3}\right)$$

Is There a Base-10 Formula for Pi?



Note that there is both a base-2 and a base-3 BBP-type formula for π^2 . Base-2 and base-3 formulas are also known for a handful of other constants.

Questions:

- 1. Is there a base-3 BBP-type formula for π ?
- 2. Is there a base-10 BBP-type formula for π ?
- 3. Is there any base-n (n \neq 2b) BBP-type formula for π ?

Answers: No. This is ruled out in a recent paper by Jon Borwein, David Borwein and Will Galway.

This does not rule out some completely different scheme for finding individual non-binary digits of π .

An Arctan Formula



$$\arctan\left(\frac{4}{5}\right) = \frac{1}{2^{17}} \sum_{k=0}^{\infty} \frac{1}{2^{20k}} \left(\frac{524288}{40k+2} - \frac{393216}{40k+4} - \frac{491520}{40k+5} + \frac{163840}{40k+8} + \frac{32768}{40k+10} - \frac{24576}{40k+12} + \frac{5120}{40k+15} + \frac{10240}{40k+16} + \frac{2048}{40k+18} + \frac{1024}{40k+20} + \frac{640}{40k+24} + \frac{480}{40k+25} + \frac{128}{40k+26} - \frac{96}{40k+28} + \frac{40}{40k+32} + \frac{8}{40k+34} - \frac{5}{40k+35} - \frac{6}{40k+36}\right)$$

A Numerical Integration Solution



Using a high-precision numerical integration program, together with PSLQ, we found that if

$$C(a) = \int_0^1 \frac{\arctan\sqrt{x^2 + a^2}}{(x^2 + 1)\sqrt{x^2 + a^2}} dx$$

Then

$$C(0) = (\pi \log 2)/8 + G/2$$

 $C(1) = \pi/4 - \pi\sqrt{2}/2 + 3\sqrt{2}/2 \cdot \arctan \sqrt{2}$
 $C(\sqrt{2}) = 5\pi^2/96$

Several general results have also been found.

Another Integral Evaluation



Recently it was found, using the Toolkit program, that if

$$C(t) = \frac{2}{\sqrt{3}} \int_0^1 \frac{1}{1-x} \log^t \left(\arctan \frac{x\sqrt{3}}{x-2} \right) dx$$

$$L(t) = \sum_{n=1}^{\infty} \left[\frac{1}{(3n-2)^t} - \frac{1}{(3n-1)^t} \right]$$

Then

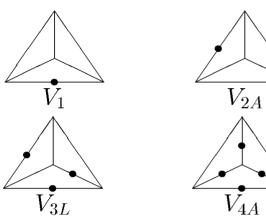
$$C(3) = \frac{1}{12} [27L(4) - 6L(2)\zeta(2) - 32\zeta(4)]$$

$$C(5) = \frac{1}{36} [891L(6) - 162L(4)\zeta(2) + 360L(3)\zeta(3) -546L(2)\zeta(4) - 928L(1)\zeta(5)]$$

$$C(7) = \frac{1}{72} [52245L(8) - 8910L(6)\zeta(2) + 18360L(5)\zeta(3) -24570L(4)\zeta(4) + 30000L(3)\zeta(5) - 37510L(2)\zeta(6) -52720L(1)\zeta(7)]$$

Evaluation of Ten Constants from Quantum Field Theory





$$V_{3L}$$

$$V_{4A}$$

$$V_{1} = 6\zeta(3) + 3\zeta(4)$$

$$V_{2A} = 6\zeta(3) - 5\zeta(4)$$

$$V_{2N} = 6\zeta(3) - \frac{13}{2}\zeta(4) - 8U$$

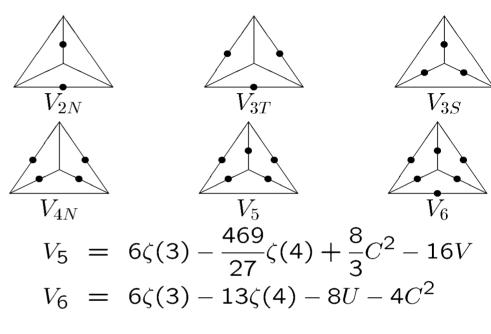
$$V_{3T} = 6\zeta(3) - 9\zeta(4)$$

$$V_{3S} = 6\zeta(3) - \frac{11}{2}\zeta(4) - 4C^{2}$$

$$V_{3L} = 6\zeta(3) - \frac{15}{4}\zeta(4) - 6C^{2}$$

$$V_{4A} = 6\zeta(3) - \frac{77}{12}\zeta(4) - 6C^{2}$$

$$V_{4N} = 6\zeta(3) - 14\zeta(4) - 16U$$



where

$$C = \sum_{k>0} \sin(\pi k/3)/k^{2}$$

$$U = \sum_{j>k>0} \frac{(-1)^{j+k}}{j^{3}k}$$

$$V = \sum_{j>k>0} (-1)^{j} \cos(2\pi k/3)/(j^{3}k)$$

PSLQ and **Sculpture**



The complement of the figure-eight knot, when viewed in hyperbolic space, has finite volume

$$V = 2.029883212819307250042...$$

Recently David Broadhurst found, using PSLQ, that V is given by a base-3 BBP-type formula:

$$V = \frac{\sqrt{3}}{9} \sum_{n=0}^{\infty} \frac{(-1)^n}{27^n} \left(\frac{18}{(6n+1)^2} - \frac{18}{(6n+2)^2} - \frac{24}{(6n+3)^2} - \frac{6}{(6n+4)^2} + \frac{2}{(6n+5)^2} \right)$$



Some Supercomputer-Class PSLQ Solutions



- Identification of B₄, the fourth bifurcation point of the logistic iteration.
 - Integer relation of size 121; 10,000 digit arithmetic.
- Identification of Apery sums.
 - 15 integer relation problems, with size up to 118, requiring up to 5,000 digit arithmetic.
- Identification of Euler-zeta sums.
 - Hundreds of integer relation problems, each of size 145 and requiring 5,000 digit arithmetic.
 - Run on IBM SP parallel system.
- Finding relation involving root of Lehmer's polynomial.
 - Integer relation of size 125; 50,000 digit arithmetic.
 - Utilizes 3-level, multi-pair parallel PSLQ program.
 - Run on IBM SP using ARPEC; 16 hours on 64 CPUs.

A Cautionary Example



$$\int_0^\infty \frac{\sin x}{x} dx = \frac{\pi}{2}$$

$$\int_0^\infty \frac{\sin x}{x} \cdot \frac{\sin(x/3)}{x/3} dx = \frac{\pi}{2}$$

$$\int_0^\infty \frac{\sin x}{x} \cdot \frac{\sin(x/3)}{x/3} \cdot \frac{\sin(x/5)}{x/5} dx = \frac{\pi}{2}$$

$$\int_0^\infty \frac{\sin x}{x} \cdot \frac{\sin(x/3)}{x/3} \cdot \frac{\sin(x/5)}{x/5} \cdots \frac{\sin(x/13)}{x/13} dx = \frac{\pi}{2}$$

but

$$\int_0^\infty \frac{\sin x}{x} \cdot \frac{\sin(x/3)}{x/3} \cdot \frac{\sin(x/5)}{x/5} \cdots \frac{\sin(x/15)}{x/15} dx$$

$$= \frac{467807924713440738696537864469}{935615849440640907310521750000} \pi$$

Another Cautionary Example



These constants agree to 42 decimal digit accuracy, but are NOT equal:

$$\int_0^\infty \cos(2x) \prod_{n=0}^\infty \cos(x/n) dx =$$
0.39269908169872415480783042290993786052464543418723...
$$\frac{\pi}{8} =$$
0.39269908169872415480783042290993786052464617492189...

Normal Numbers



- A number is b-normal (or "normal base b") if every string of m digits in the base-b expansion appears with limiting frequency b^{-m}.
- Using measure theory, it is easy to show that almost all real numbers are b-normal, for any b.
- Widely believed to be b-normal, for any b:
 - $\pi = 3.1415926535...$
 - e = 2.7182818284...
 - Sqrt(2) = 1.4142135623...
 - Log(2) = 0.6931471805...
 - All irrational roots of polynomials with integer coefficients.

But to date there have been NO proofs for any of these.

Proofs have been known only for contrived examples, such as C = 0.12345678910111213...

A Connection Between BBP Formulas and Normality



- In 2001 Richard Crandall and I found a connection between BBP-type formulas and a class of iterative sequences. In particular, we found:
- A mathematical constant given by a BBP-type formula is b-normal if and only if an associated iterative sequence is equidistributed in the unit interval.

This result relies crucially on the BBP formula for π and some other similar formulas, many of which were discovered using PSLQ computations.

Example: Log_e 2



Consider the sequence (x_n) given by $x_0 = 0$ and

$$x_n = \{2x_{n-1} + 1/n\}$$

Successive values of (x_n) appear to dance about randomly in the interval (0, 1):

0.0000, 0.5000, 0.3333, 0.9167, 0.0333, 0.2333, 0.6095, 0.3440,

0.7992, 0.6984, 0.4877, 0.0588, 0.1945, 0.4605, 0.9876, 0.0378,

0.1344, 0.3243, 0.7012, 0.4524, 0.9524, 0.9502, 0.9439, 0.9295, ...

If it can be shown that (x_n) are equidistributed in the unit interval, then this would suffice to establish that log 2 is 2-normal.

The Iterative Sequence for Pi



The associated sequence for π is:

$$x_n = \left\{ 16x_{n-1} + \frac{120n^2 - 89n + 16}{512n^4 - 1024n^3 + 712n^2 - 206n + 21} \right\}$$

Just as in the case of log 2, if it can be established that (x_n) is equidistributed in (0, 1), then it would follow that π is 16-normal, and hence 2-normal also.

Curious fact:

Define the sequence (y_n) by $y_n = \{16 \ x_n\}$. Then (y_n) appears to perfectly generate the hexadecimal expansion of π . We have verified this by computer to over 1,000,000 digits.

A Class of Provably Normal Constants



Crandall and I have also shown (unconditionally) that an infinite class of mathematical constants is normal, including

$$\alpha_{2,3} = \sum_{k=1}^{\infty} \frac{1}{3^k 2^{3^k}}$$

$$= 0.041883680831502985071252898624571682426096..._{10}$$

$$= 0.0AB8E38F684BDA12F684BF35BA781948B0FCD6E9E0..._{16}$$

 $\alpha_{2,3}$ was proven 2-normal by Stoneham in 1971, but we have extended this to the case where (2,3) are any pair of relatively prime integers. We also extended to uncountably infinite class, as follows [here r_k is the k-th bit of r in (0,1)]:

$$\alpha_{2,3}(r) = \sum_{k=1}^{\infty} \frac{1}{3^k 2^{3^k + r_k}}$$

The Iterative Sequences Associated with Alpha Constants



The iterative sequence associated with the $\alpha_{2,3}$ constant has a special structure:

```
0, 0, 0, 1/3, 2/3, 1/3, 2/3, 1/3, 2/3, 4/9, 8/9, 7/9, 5/9, 1/9, 2/9, 4/9, 8/9, 7/9, 5/9, 1/9, 2/9, 4/9, 8/9, 7/9, 5/9, 1/9, 2/9, 13/27, 26/27, 25/27, 23/27, 19/27, 11/27, 22/27, 17/27, 7/27, 14/27, 1/27, 2/27, 4/27, 8/27, 16/27, 5/27, 10/27, 20/27, 13/27, 26/27, 25/27, 23/27, 19/27, 11/27, 22/27, 17/27, 7/27, 14/27, 1/27, 2/27, 4/27, 8/27, 16/27, 5/27, 10/27, 20/27, 13/27, 26/27, 25/27, 23/27, 19/27, 11/27, 22/27, 17/27, 7/27, 14/27, 1/27, 2/27, 4/27, 8/27, 16/27, 5/27, 10/27, 20/27, etc.
```

Note that each set of numerators consists of precisely those integers relatively prime to the denominator.

The "Hot Spot" Lemma: The Key to Proving that Pi is 2-Normal?



Hot spot lemma: α is b-normal if and only if there is some C>0 such that for any subinterval [c,d) of [0,1) it is true that

$$\limsup_{n>0} \frac{\#_{0 \le j < n}(\{b^j \alpha\} \in [c,d))}{n} \le C(d-c)$$

In other words, if α is *not* b-normal, then there must be strings that appear in the base-b expansion of α arbitrarily more often than their "natural" frequency.

This lemma can be used to produce a very simple proof that $\alpha_{2,3}$ is 2-normal.

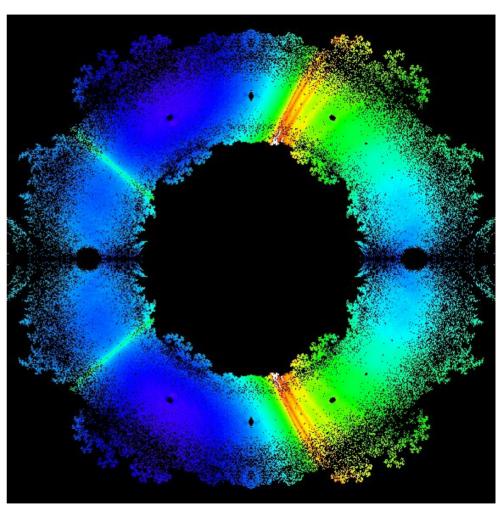
Perhaps also for log 2 and π ?

An Unsolved Question of Experimental Mathematics



This is a plot of all roots of polys with coefficients 1 or -1 up to degree 18, colored by sensitivity of the polys to variation around the values of the zeros.

The bands, clearly visible in the plot, are unexplained.



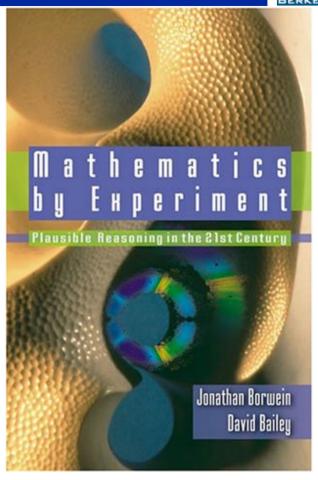
Two New Books on Experimental Mathematics



Vol. 1: Mathematics by
Experiment: Plausible
Reasoning in the 21st
Century [now available]

Vol. 2: Experiments in Mathematics: Computational Paths to Discovery [soon]

Authors: Jonathan M Borwein and David H Bailey, with Roland Girgensohn for Vol. 2.



A "Reader's Digest" condensed version is available FREE at http://www.expmath.info